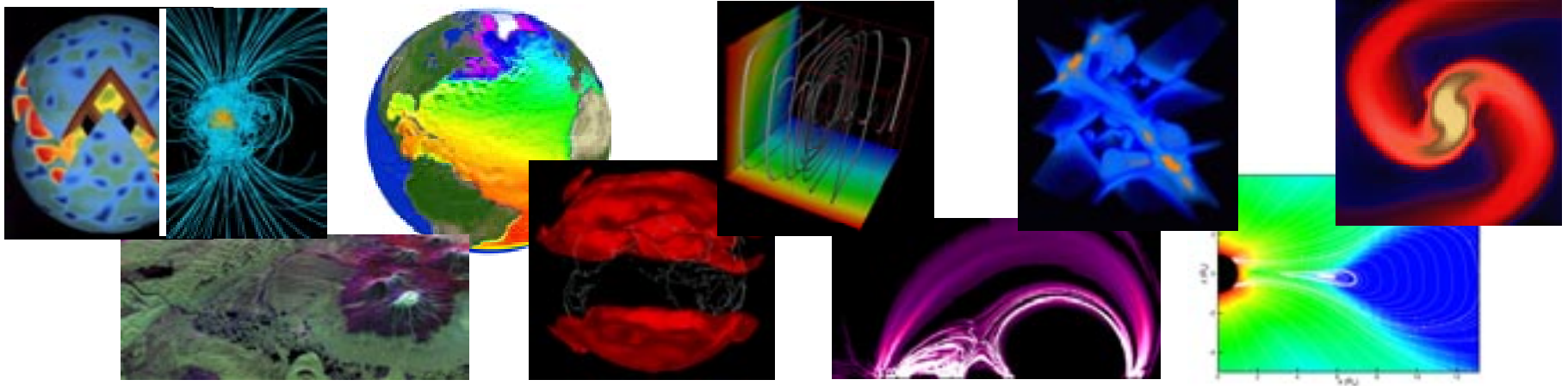


NASA Earth Science Technology Office (ESTO)

Computational Technologies (CT) Project

Formerly HPCC Earth and Space Science (ESS) Project

Project Briefing to ESTO Technology Strategy Team



Jim Fischer/GSFC, Project Manager
Robert Ferraro/JPL, Associate Project Manager

☐ November 28, 2001
☐ Hampton, Virginia



Goal, Objectives, and Legacy

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Goal

Demonstrate the power of high-end and scalable cost-effective computing environments to further our understanding and ability to predict the dynamic interaction of physical, chemical, and biological processes affecting the Earth, the solar-terrestrial environment, and the universe.

- HPCC Program Plan - June 2000

Objectives

- **Customer Impact** - *Infuse* high performance computing technologies into mission critical stakeholder Enterprise/Office processes, document discernible improvements in the stakeholders' *processes* and, if possible, document discernible improvements in the final *products* as a result.
- **Computational and Communication Performance** - Dramatically increase the computer and communication performance *available for use* in meeting NASA mission requirements.
- **Interoperability** - Dramatically increase the interoperability of *application and system software* operating on high-performance computing and communications systems available for use in meeting NASA mission requirements.
- **Portability** - Dramatically improve the portability of *application software and data* to new or reconfigured high-performance computing and communications systems available for use in meeting NASA mission requirements.
- **Customer Usability** - Dramatically improve the usability of high-performance computing and communications *tools and techniques* available for use in meeting NASA mission requirements.

Code Y Legacy

Infrastructure of high performance interoperating Earth System Modeling research codes supporting NOAA, NSF, DOE, DOD and NASA.





ESS Implementation Approach (FY92-99)

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ESS Round-1 Grand Challenge Investigations (FY92-95)

- In response to **NRA**-OSSA-92, and following a full peer review, NASA HQ selected 8 Grand Challenge teams of Earth and space scientists and 21 Guest Computational Investigators.
- Science related performance metrics with baselines were established and measured.
- Final Report: <http://sdcd.gsfc.nasa.gov/ESS/sciteam1.report/sciteam1.gc.html>
- **The absence of a large ESS computing system and the use of grants as the award vehicle inhibited ability to achieve stated goals.**

ESS Round-2 Grand Challenge Investigations (FY96-00)

- Structured differently from Round-1 to overcome shortcomings in that approach.
- Investigators and a Testbed were acquired through a single Cooperative Agreement Notice (**CAN**-21425/041)
- CAN was structured to incentivize strong collaboration between the testbed vendor and the Investigators to meet aggressive joint performance milestones.
- Signed cooperative agreements worth \$12.6M with 9 Grand Challenge Teams to achieve Project milestones of 10, 50 and 100 Gflop/s sustained on their scientific codes.
- Signed a \$13.2M cooperative agreement with SGI/Cray to place a large scalable parallel Testbed (for the Round-2 Investigators, the broader NASA science community, and the HPCC CAS Project).
- Every payment was tied to achievement of one of 117 negotiated milestones.
- **This approach produced the desired results.**

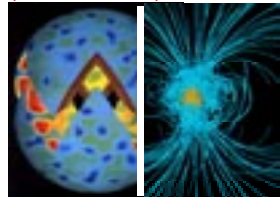


Status Report on ESS Round-2 Investigator Performance Milestones

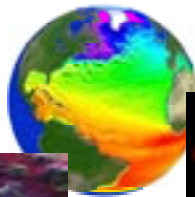
Round-2 ESS Grand Challenge Investigators

\$12.6M over 3 years

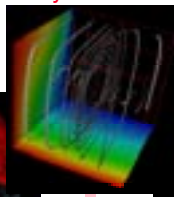
Simulations of the Earth's Core and Mantle Dynamics
(P.Olson/JHU)



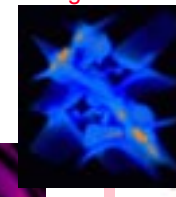
Atmosphere/Ocean Dynamics and Tracers Chemistry
(R.Mechoso/UCLA)



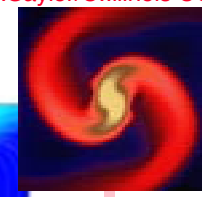
Rayleigh-Benard-Marangoni Problems in a Microgravity Environment
(G.Carey/U.Texas Austin)



Turbulent Convection and Dynamos in Stars
(A.Malagoli/U.Chicago)



Relativistic Astrophysics and Gravitational Wave Astronomy
(P.Saylor/U.Illinois UC)



SAR Interferometry and Imaging Science
(D.Curkendall/JPL)



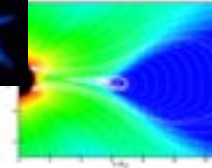
Four Dimensional Data Assimilation
(P.Lyster/U.Maryland)



Solar Activity and Heliospheric Dynamics
(J.Gardner/NRL)



Multiscale Modeling of the Heliosphere
(T.Gombosi/U.Michigan)



Performance Milestone Achievements

CT7 GC5	100 Gigaflap/s*	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE
CT4 GC4	50 Gigaflap/s*	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE
GC2	10 Gigaflap/s*	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE	4 NHSE

*or x over baseline

Collaborations to restructure specified Investigator codes to achieve milestone performance

"NHSE" indicates codes that have been made available to the scientific community via the National HPCC Software Exchange - <http://www.nhse.org/>

1024 Processor SGI/Cray T3E at GSFC

512 processors are used by ESS and
512 processors are used by NSIPP

\$13.2M over 3 years

50 Gigaflap/s-Sustained Testbed

448 Gflop/s on LINPACK
#1 in NASA
#3 in Earth Science
#10 in the world
(circa 1998)



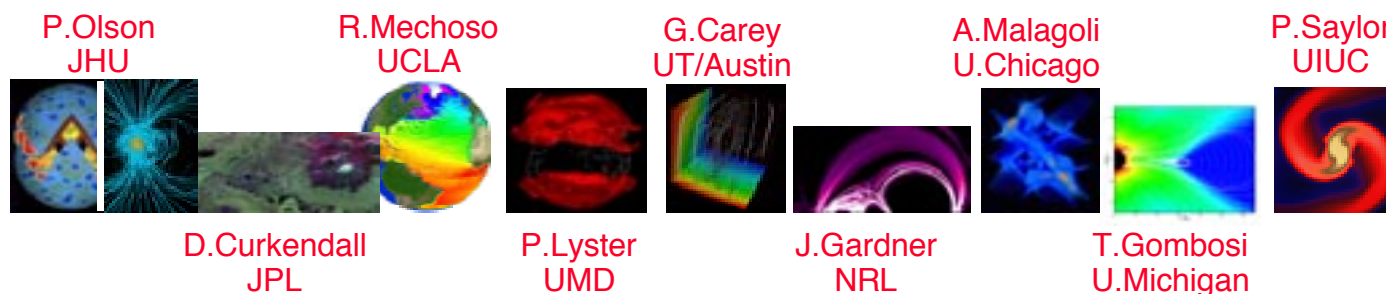
50 Terabyte tape silo



Center-based Support for Round-2 Teams

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Parallelization
& Optimization

Software
Products

Visualization
Products

Networking
Research

4	4	4	4	4	4	4	4	4
	4	4				4		
4	4	4	4	4	4	4		4
	4		4		4	4		





Three-Dimensional Spherical Simulations of Earth's Core and Mantle Dynamics

Peter Olson, Johns Hopkins University, PI

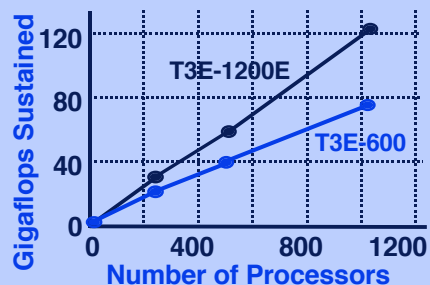
<http://www.jhu.edu/~eps/geoplabs/nasa3/start.html>

Goal: Simulate the chaotic processes that drive the evolution of the planet's interior, and in turn shape its surface, over timescales ranging from hundreds to millions of years.

TERRA is a 3D spherical finite element mantle dynamics code, developed by John Baumgardner, LANL, and his collaborators.

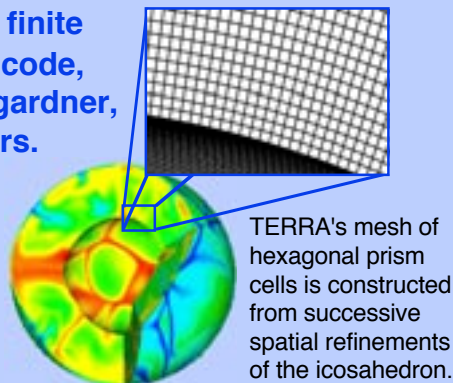
TERRA treats the silicate rock of the Earth's mantle as a non-linear viscous fluid and solves the Navier-Stokes equations for the motions that arise from variations in temperature and density.

- Achieved, in Round-2, major algorithmic advances to enable TERRA to treat extreme local variations in material properties.
- Increased the speed of TERRA by a factor of 125.
- Applied TERRA to several fundamental science questions concerning the history and dynamics of the Earth.



TERRA sustained 121 Gigaflops on 1024 processors of a CRAY T3E-1200E, and 10 Gigaflops on 128 processors of a 350Mhz Pentium-II Linux cluster.

Prior to ESS support, TERRA was baselined in 1995 at 0.96 Gigaflops on a Cray T3D.



TERRA offers a powerful simulation capability to apply the vast datasets from surface geology to constrain and test models of a planet's internal dynamics and history, i.e., advance tangibly the emerging synthesis of geology and geophysics.

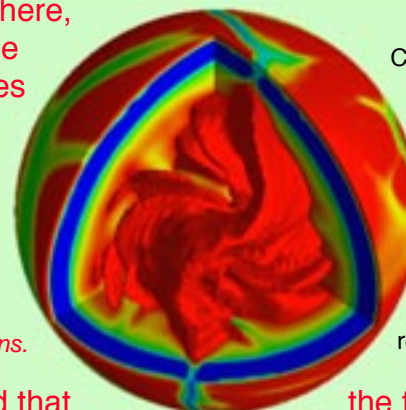
The new ability to obtain platelike behavior directly from silicate rheology has opened the door to new discoveries about the Earth's interior

Recent TERRA simulations confirm that the asthenosphere, a low viscosity zone just below the plates in the Earth, plays a crucial role in stabilizing a plate tectonics style of mantle dynamics.

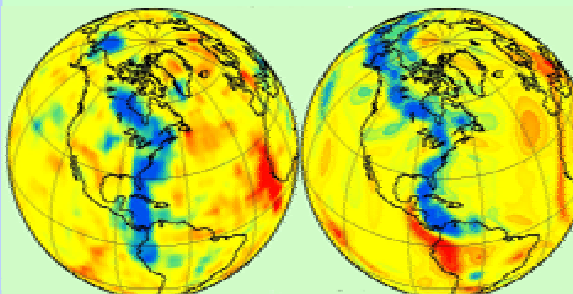
Required $\sim 5 \times 10^{15}$ floating point operations.

Rheology has to do with material deformation properties.

Colors represent viscosity, increasing from blue to red. Note high viscosity surface layer overlying low viscosity asthenosphere. The red isosurface represents cold high viscosity plate material from the surface that is sinking into the deeper mantle. The grid for this case has 10,649,730 cells and a spatial resolution of about 50 km.



TERRA discovered that the tectosphere, a keel-like feature beneath much of the continental area, plays only a very small role in the overall motions of the tectonic plates.



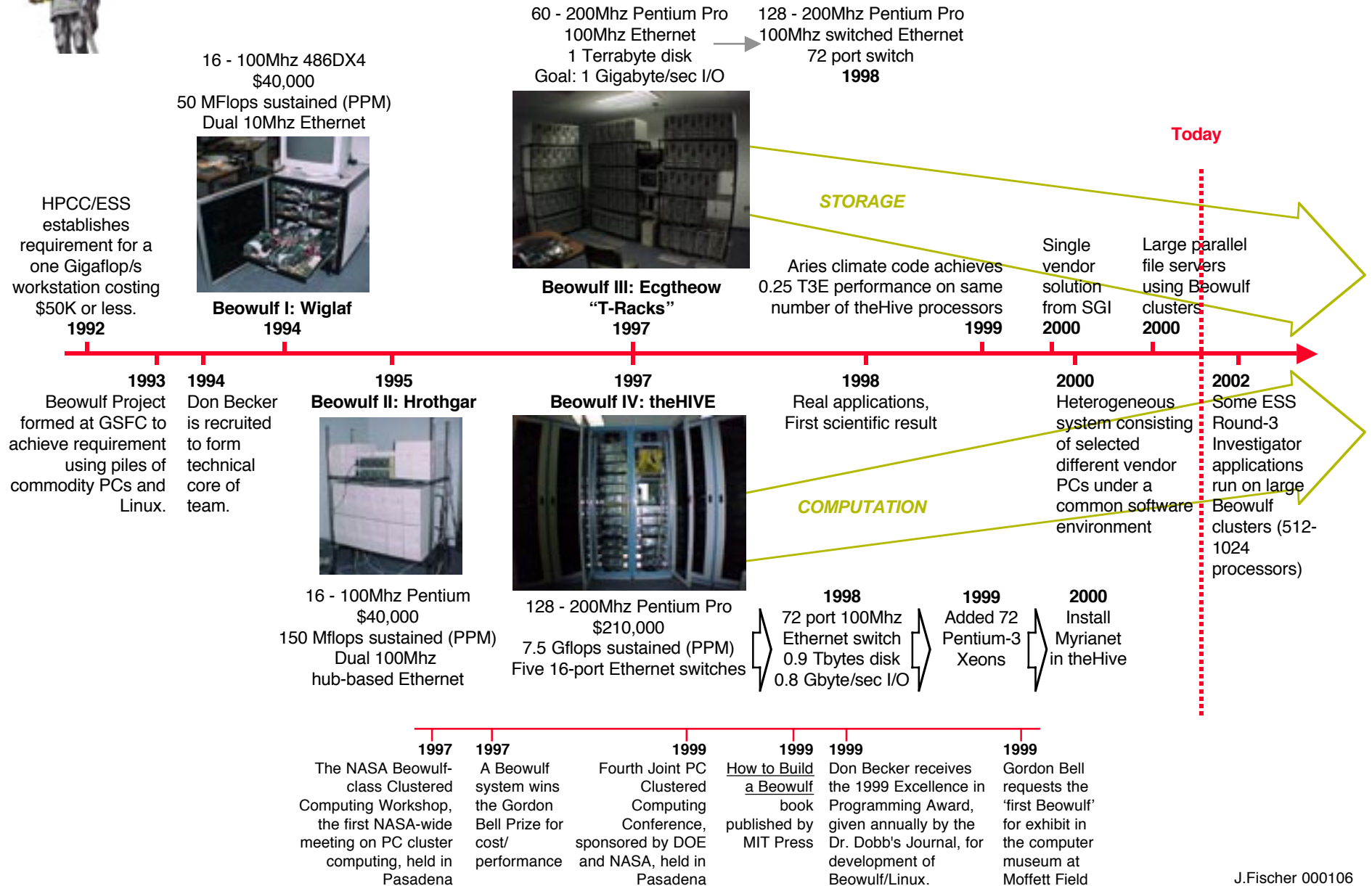
Plot on left is seismic image of Farallon slab (blue). Right plot shows (blue) subducted material in a TERRA simulation based on plate motion history applied as a surface boundary condition.

TERRA demonstrated for the first time the combination of 3D seismic tomography models and 3D geodynamic modeling could improve the accuracy of the plate motion models, here illustrated for the subducted Farallon slab beneath North America.



The Beowulf Project - the GSFC-centric time line

<http://beowulf.gsfc.nasa.gov/>





Tenth NASA Summer School in High Performance Computational Earth and Space Sciences

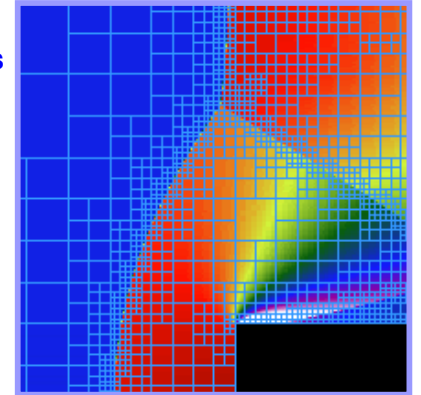
July 10 - 28, 2000

Goal: Train the next generation of computational Earth and Space scientists in massively parallel techniques and algorithm development.

Format: Three weeks of intensive lectures and lab sessions hosted at GSFC by the NASA Center for Computational Sciences.

Curriculum

- Finite Volume Methods
- Shock Capturing Methods
- Finite Element Methods
- Spectral and Spectral-Element Methods
- Particle Methods
- Methods for Atmospheric and Ocean Flows
- Software Engineering



Instruction

Lecturers included the ESS Inhouse Team of computational scientists:

- Steven Zalesak, lead lecturer - GSFC
- Phillip Merkey - Michigan Tech Univ.
- Tom Clune - SGI
- Spencer Swift - SGI
- Peter MacNeice - Drexel University
- Anil Deane - University of Maryland
- Kevin Olson - University of Chicago
- Jay Boris - NRL (canceled due to illness)
- Max Suarez - GSFC
- Tarek El-Ghazawi - George Mason Univ.
- Rainald Lohner - George Mason Univ.

Students

Sixteen Doctoral Candidates selected through a national solicitation.

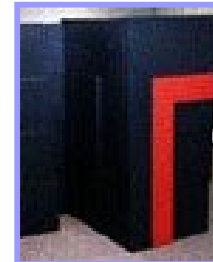


158 alumni over 10 years
including a number of members of
ESS Investigator Teams.

Parallel Computing Platforms

Lab sessions in parallel code development for selected high performance computers.

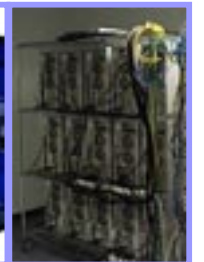
Cray
T3E-600



Origin
2000



Linux cluster
of PCs





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Round-3





Implementation Approach (FY01-04)

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Areas of Emphasis *Derived from the NASA Science Community*

- Improve **software engineering environments** to manage the complexity of evolving high-performance modeling and analysis software systems.
- Bring about **interoperability** of high-performance code components within and among related research groups.
- Design software for rapid **portability and performance optimization** of applications among the variety of high-performance architectures.
- **Improve** key high-performance codes in units of quality valued by the science community or flight projects.
- Achieve interoperability of application components and high performance simultaneously.
- Provide key **middleware** software components compatible with the software interoperability standards.
- Provide more capable and cost-effective **computing systems** and environments to carry out the research that addresses the above requirements.
- Provide **visualization tools** capable of handling the data volumes associated with teraflops systems and that are accessible from remote locations.





Implementation Approach (FY01-04)

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Round-3 builds on strengths of Round-2:

- Acquire a third round of **Investigator Teams** using a CAN and full peer review
- Negotiate **performance based milestones** into 3-year cooperative agreements
- **Link** Project milestone achievement to Team milestone achievement
- Provide access to high end **computing systems** to support Team milestone achievement
- **Link** computing system vendor success to Investigator Team success

And has new features:

- Emphasize Round-3 Investigations that:
 - Are **relevant** to NASA science mission objectives (Codes Y, S, U and M)
 - **Incorporate NASA data** to understand phenomena or to test and evaluate the models being developed
 - Build **interoperable community capabilities** through software frameworks or other proposed techniques
 - Aim to **support** a broad user community in their field
- Have Headquarters release the CAN and provide the Selection Official
- Use **science based metrics** (not gigaflops) for Investigator code improvements
- Utilize **less expensive** commodity based computing systems when feasible
- **Link** GSFC and JPL center-based R&D activities to Team success through shared milestones
- Carry out additional **supporting solicitations** shaped by Investigator needs





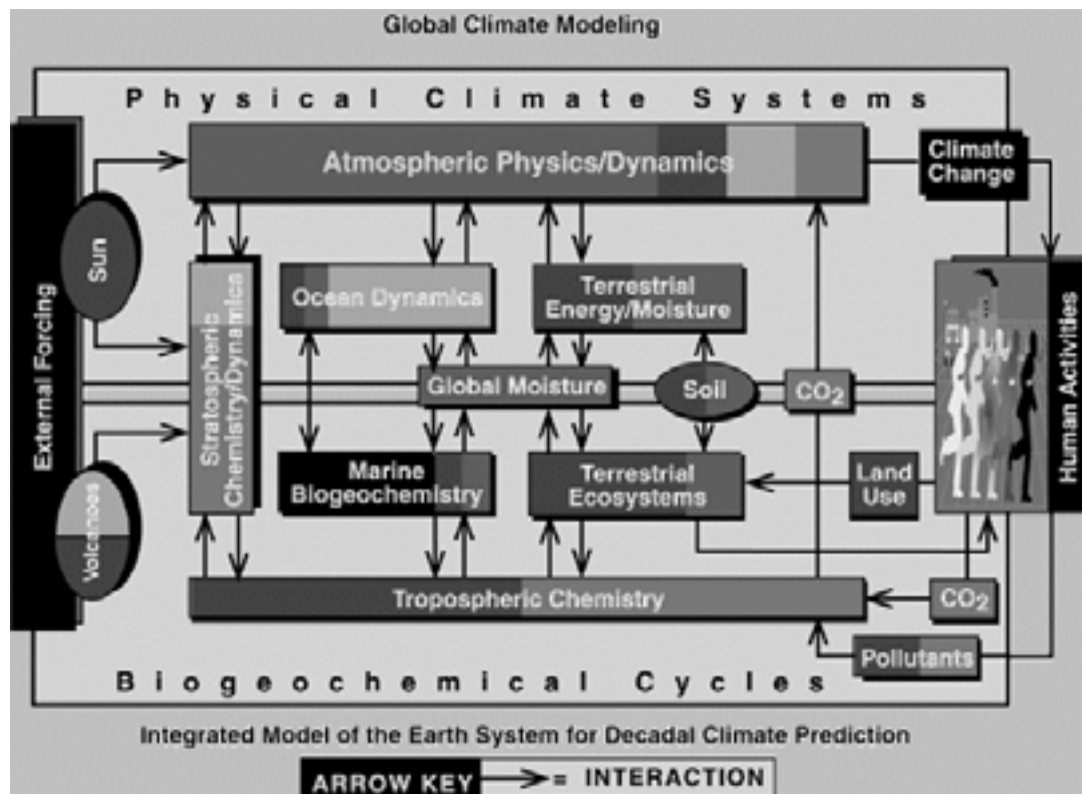
The Earth Science Enterprise Mission

Develop a scientific understanding of the Earth System and its response to natural and human-induced changes to enable improved prediction of climate, weather, and natural hazards for present and future generations.

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“Unequivocal statements ... to policy makers will undoubtedly be based on climate models that have demonstrably improved scientific parameterizations and greater physical fidelity.” - *Dr. Tim Killeen, Director NCAR*



The Earth Science Enterprise needs to achieve interoperation of many model systems

How can CT enable this bold vision?

The Earth System and Its Interactions
from page 3 of the
Earth Science
Strategic Enterprise
Plan 1998-2002



"Insufficient human and computational resources are being devoted to high-end, computer intensive, comprehensive modeling, perhaps, in part, because of the **absence of a nationally coordinated modeling strategy."**

1998 National Research Council report

"Capacity of U.S. Climate Modeling to Support Climate Assessment Activities"

**The Round-3 CAN
was developed to
address this issue.**

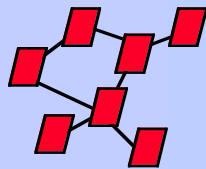


Provide a Viable Earth System Modeling Framework

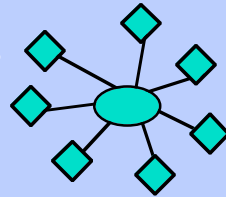
Current Situation:

Even though several major atmospheric models employ modern software engineering involving frameworks, none of the frameworks interoperate.

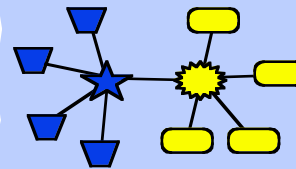
Model A



Model B



Model & Analysis C

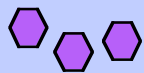


Running under various systems

- Flux Coupler (NCAR)
- GEMS (GSFC)
- Flexible Modeling System (GFDL)
- Data Broker (UCLA)
- ... and others

Making it very hard for:

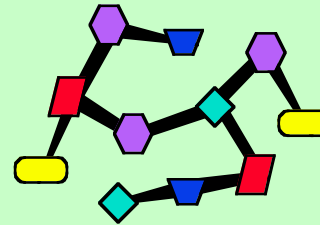
- Models to incorporate advances from outside their framework;



3rd party objects

- Other intellectual communities to help the modeling communities.

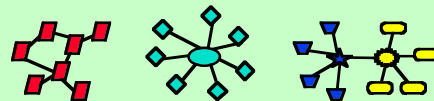
The need is for a Common Framework Infrastructure



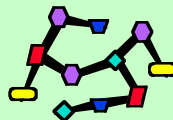
Some significant Code Y communities such as weather and climate modeling are ready to adopt a common infrastructure.

ESS intends to facilitate this evolutionary step

in Round-3 for a key Code Y community.



ESS Round-3 CAN



Earth System Modeling Framework

There is significant risk: Mitigation:

- 1) That high performance and interoperability will not be achieved together.
 - 2) That a sub-critical mass of the community will participate in the design and convert to it.
- 1) Milestones must be constructed to require both.
 - 2) Other solicitations must help to populate the framework.



The ESMF Will Assist the U.S. Climate Research Community to Advance by:

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- Reducing redundant effort and maximizing the time spent by scientists and software developers in producing research products rather than computational infrastructure;
- Strengthening communication and collaboration among diverse groups of Earth system researchers, enhancing the community's ability to organize to address specific issues;
- Strengthening the links between the weather forecasting and climate modeling communities and allowing testing of climate models in assimilation and forecast systems;
- Increasing the scalability of climate models, allowing higher resolution and/or longer simulations on highly parallel US supercomputers;
- Increasing the portability of climate models to allow groups to easily take advantage of computational resources wherever available and regardless of hardware;
- Simplifying the construction of climate models and the exchange and incorporation of new submodels to allow a more complete description of the climate system;

Provided by Dr. Tim Killeen, Director NCAR



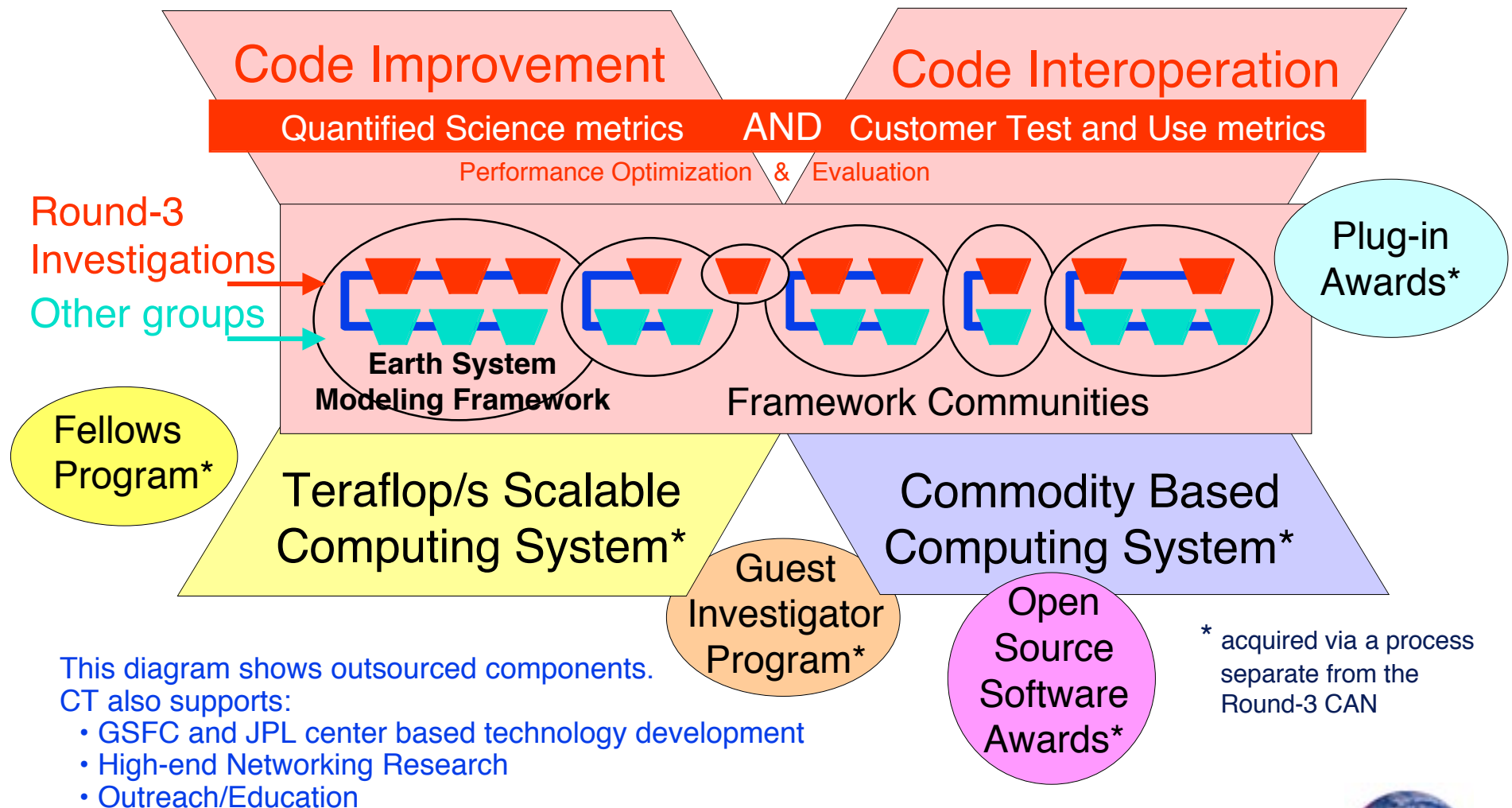


Round-3 Components

CAN components shown in red

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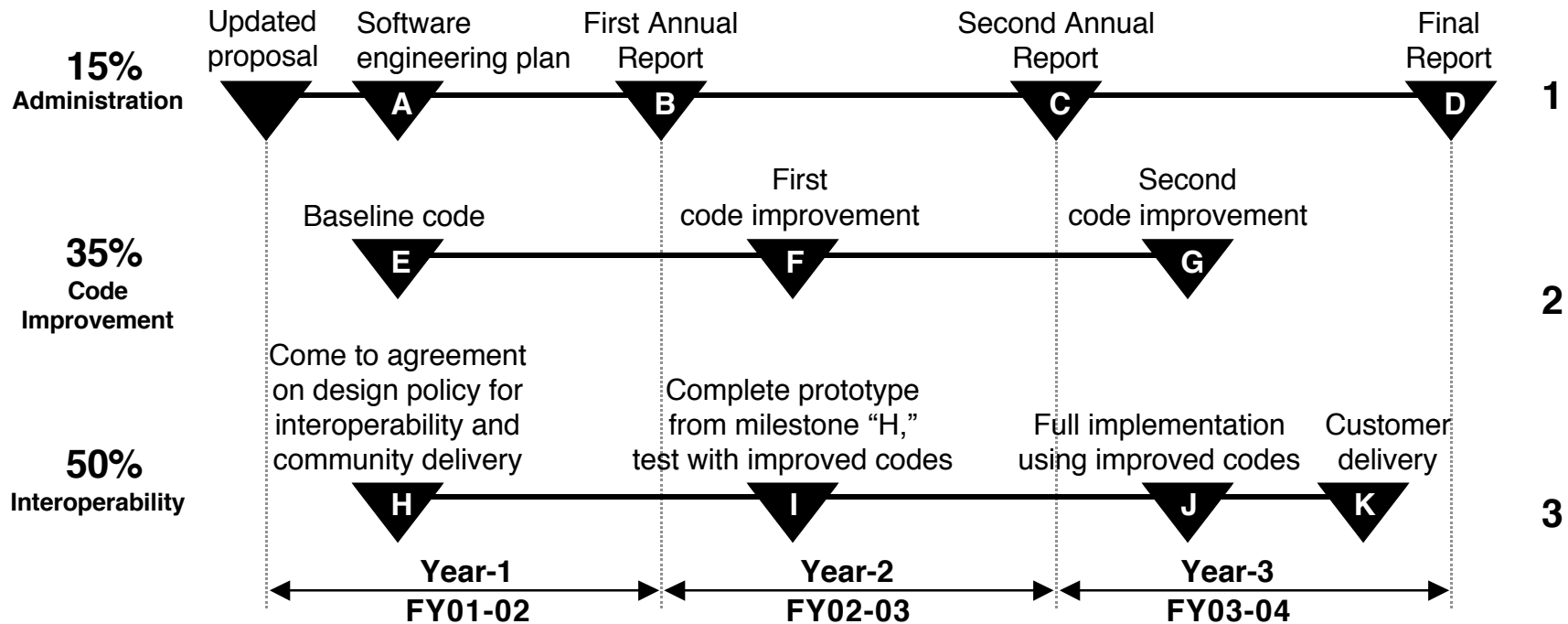




Milestone Template in CAN

CAN-00-OES-01
“Increasing Interoperability and
Performance of Grand Challenge
Applications in the Earth, Space,
Life and Microgravity Sciences”

Required milestones (11)



Optional Milestones (up to 2)

Joint collaborations between Investigator Teams and ESS technology groups at GSFC, JPL or ARC.

- a) Parallel Adaptive Mesh Refinement pkg augmentation
- b) Visualization research
- c) Mass storage research
- d) Networking research

Encourage use of PC clusters by Investigator Institutions

- e) Install a PC cluster at an Investigator’s home site
- f) Achieve code improvement milestone on a PC cluster

Assist spin-offs of ESS technologies

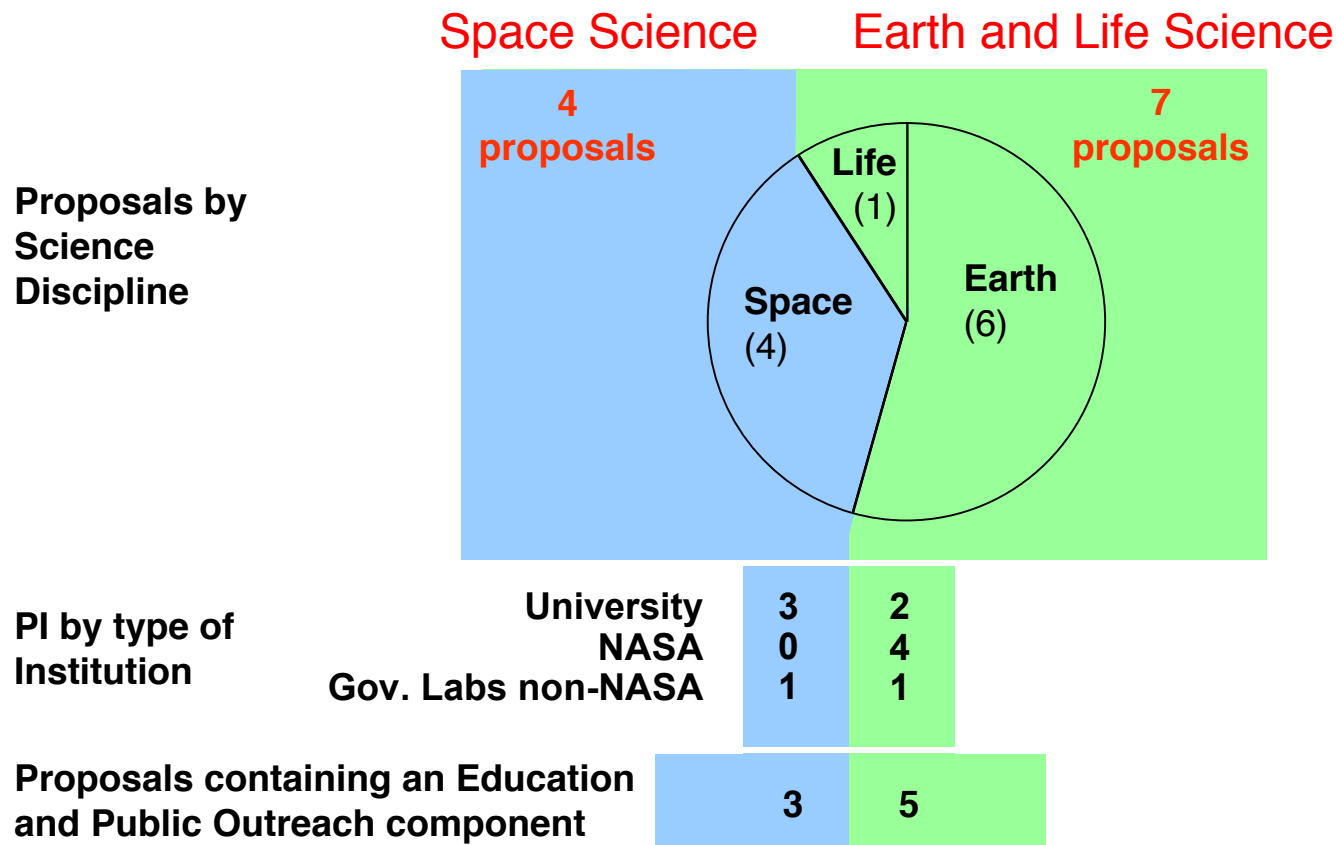
- g) Software tools
- h) Education and Public Outreach (E/PO)
- i) Broader technology transfer and access (applications)

Technology Collaborations



Profiles of Proposals Selected for Negotiations

CAN-00-OES-01
“Increasing Interoperability and
Performance of Grand Challenge
Applications in the Earth, Space,
Life and Microgravity Sciences”



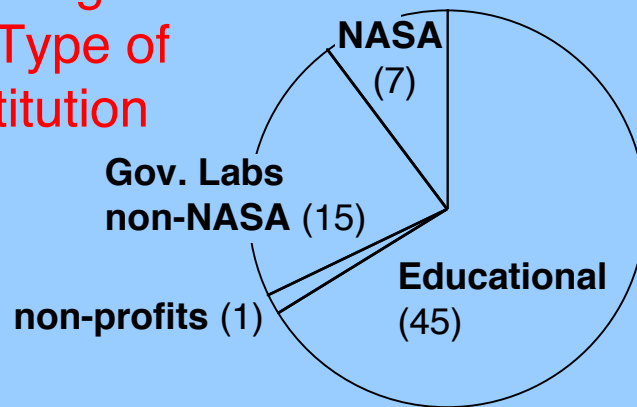


Profiles of Proposals Selected for Negotiations

CAN-00-OES-01
“Increasing Interoperability and
Performance of Grand Challenge
Applications in the Earth, Space,
Life and Microgravity Sciences”

Space Science

Investigators by Type of Institution



Software Engineers (9) Scientists (13)

Computer
Scientists (6)

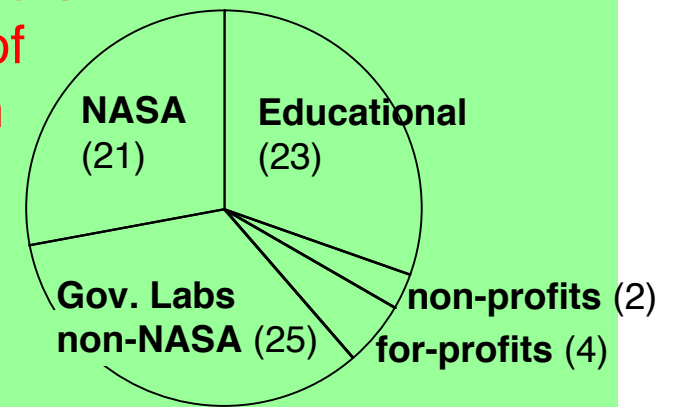
Other (1)

Computational
Scientists (39)

Investigators by Interest

Earth and Life Science

Investigators by Type of Institution



Software Engineers (8)

Scientists (10)

Computer
Scientists (12)

Other (1)

Computational
Scientists (46)

Investigators by Interest



Round-3 Awardees for the Earth System Modeling Framework

Anticipated total funding level of \$9.8M over 3 years

CAN-00-OES-01
“Increasing Interoperability and Performance of Grand Challenge Applications in the Earth, Space, Life and Microgravity Sciences”

T. Killeen/NCAR

Negotiation in Progress

Part I: Core Earth System Modeling Framework Development

Expected outcome: Infrastructure to enable the interoperability of Earth System Model components from across the Earth modeling community on high end computing platforms.

J. Marshall/MIT

Negotiation in Progress

Part II: Modeling Applications for the Earth System Modeling Framework

Expected outcome: Integration of the major US Climate Models into the Earth System Modeling Framework

A. da Silva/GSFC

Negotiation in Progress

Part III: Data Assimilation Applications for the Earth System Modeling Framework

Expected outcome: Atmospheric and Ocean data assimilation systems integrated into the Earth System Modeling Framework.





Round-3 Awardees in Earth Science

CAN-00-OES-01
“Increasing Interoperability and
Performance of Grand Challenge
Applications in the Earth, Space,
Life and Microgravity Sciences”

Anticipated total funding level of \$6M over 3 years

A. Donnellan/JPL *Negotiation Complete*

Numerical Simulations for Active Tectonic Processes

Expected outcome: Realistic Modeling of crustal fault interactions based on observational data.

P. Houser/GSFC *Negotiation Complete*

Land Information Systems

Expected outcome: Framework for the assimilation of land data observations into land surface models to study and predict the regional and global water cycle

C.R. Mechoso/UCLA *Negotiation Complete*

Atmosphere-Ocean Dynamics and Tracer Transport

Expected outcome: ESMF components for better understanding of the El Niño/Southern Oscillation.

J. Schnase/GSFC *Negotiation in Progress*

Biotic Prediction: HPCC Infrastructure for Public Health and Environmental Forecasting

Expected outcome: Infrastructure for modeling the changing geospatial distribution of the living components of the Earth environments.





Round-3 Awardees in Space Science

CAN-00-OES-01
“Increasing Interoperability and
Performance of Grand Challenge
Applications in the Earth, Space,
Life and Microgravity Sciences”

Anticipated total funding level of \$7M over 3 years

T. Gombosi/U.Mich *Negotiation Complete*

A High-Performance Adaptive Simulation Framework for Space-Weather Modeling (SWMF)

Expected outcome: Real time space weather prediction capability based on solar observation.

P. Saylor/U.Illinois *Negotiation Complete*

Development of an Interoperability Based Environment for Adaptive Meshes (IBEAM) with Applications to Radiation-Hydrodynamic Models of Gamma-Ray Bursts

Expected outcome: Understanding of observational data from gamma ray bursts.

T. Prince/Caltech *Negotiation Complete*

High-Performance Cornerstone Technologies for the National Virtual Observatory

Expected outcome: Enabling networking and computational technologies for the NVO.

P. Colella/DoE/LLNL *Negotiation Complete*

A C++ Framework for Block-Structured Adaptive Mesh Refinement Methods

Expected outcome: Computational technologies for multi-scale modeling of astrophysical and microgravity phenomenon.

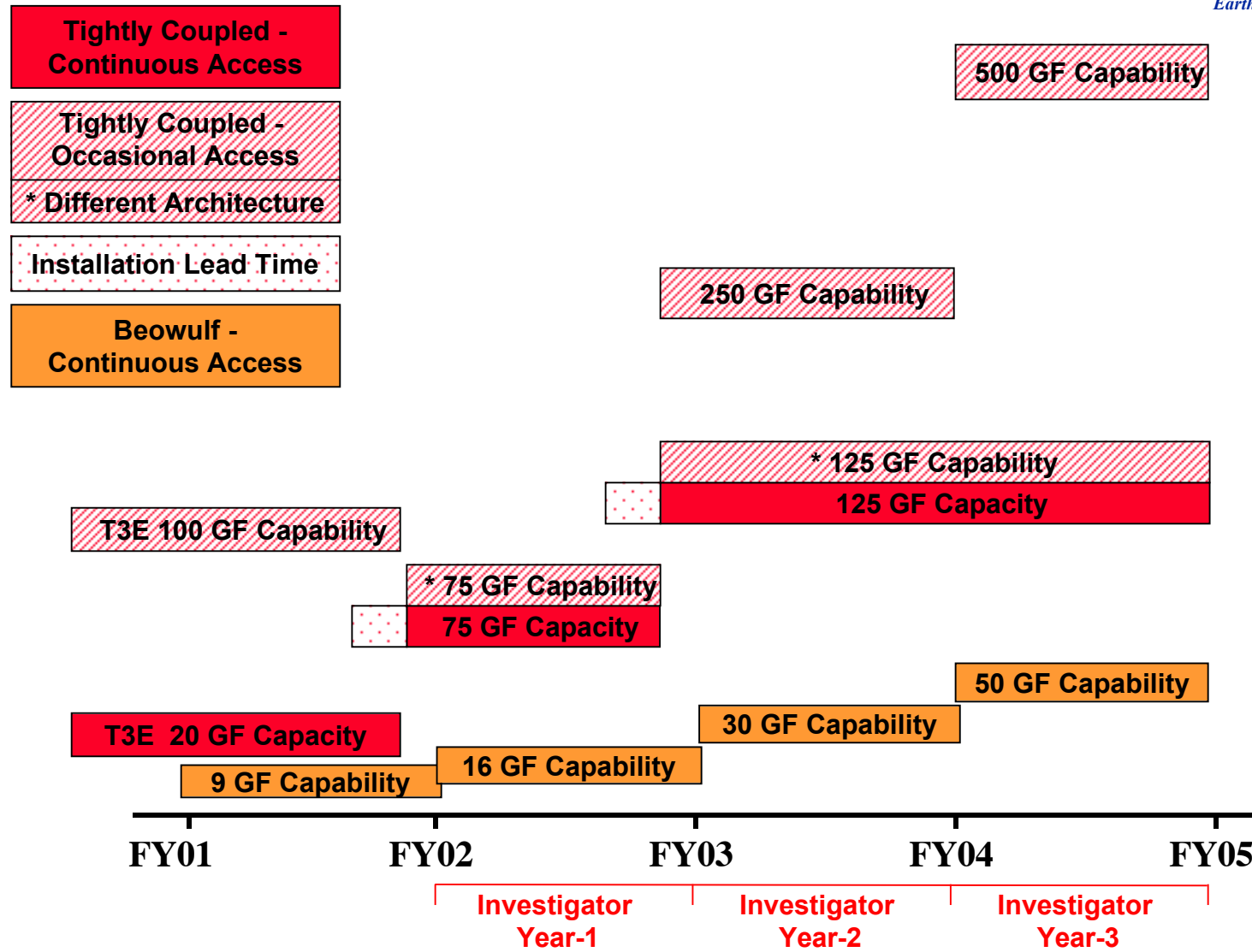




Round-3 Computing System Requirements

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Center-based support for the Round-3 Teams

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Area of Support	Principal Investigator										
	Gombosi	Saylor	Colella	Prince	Killeen	Marshall	da Silva	Donnellan	Mechoso	Houser	Schnase
Software Engineering											
Software engineering guidance	X	X	X	X	X	X	X	X	X	X	X
ESMF Risk Assessment and Mitigation					X	X	X		X	X	
Software Products											
Paramesh (structured AMR package)		X									X
Pyramid (unstructured AMR package)								X			
Parvox (visualization of very large data sets)				X				X			
Plug-in Awards	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd
National HPCC Software Exchange	X	X	X	X	X	X	X	X	X	X	X
Computing Systems											
High Performance Computing System access and data storage	X	X	X	X	X	X	X	X	X	X	X
PC Cluster access	X	X							X	X	X
Improve Open Source Software for PC Clusters	X	X							X	X	X
PC Cluster Pathfinding	X	X							X	X	X
Performance optimization	X	X	X	X	X	X	X	X	X	X	X
High performance networking										X	
Evaluation support	X	X	X	X	X	X	X	X	X	X	X
Visualization services	X	X	X	X	X	X	X	X	X	X	X
Education and Outreach											
Summer School in High Perf computational science	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd	tbd
GSRP Fellow		X		tbd				tbd	tbd	X	tbd
Information Officer	X	X	X	X	X	X	X	X	X	X	X
E/PO oversight	X			X	X	X	X	X		X	



Backups





Synthetic Aperture Radar (SAR) Interferometry and Imaging Science

David Curkendall, JPL

<http://alphabits.jpl.nasalgov/SAR/>

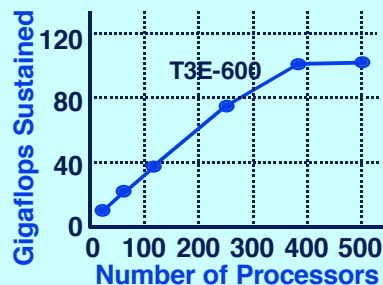
Goal: Use multiple supercomputers to process and visualize satellite-collected synthetic aperture radar data to allow close monitoring of regional changes in alpine glaciers, plate tectonics, and rain forests.

Scalable Synthetic Aperture Radar (SAR) Processor

Parallelized and made 'MPI portable' both SIR-C and the Repeat Orbit Interferometer (ROI) software processors

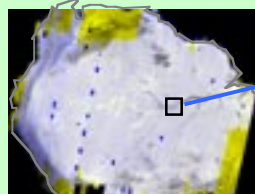
Software successfully tested on the Cray T3D and T3E, SGI Origin, HP Exemplar, and SGI workstations.

- The software turns raw data into interferometric products on a Cray T3E at a sustained raw input data rate of 14.9 Megabytes/sec.
- This throughput is 50 times greater than the 1995 baseline for just the image formation steps of 0.29 Megabytes/sec.



Large Scale Mosaic software

Developed Digital Light Table (DLT) and mosaicking software to support classification, verification and display of Terabyte images - demonstrated on 200 Gigabyte datasets.



Mosaicked three thousand JERS-1 images into a seamless dual Wet and Dry Season Portrait of the entire Amazon rainforest.

For the first time we can snapshot regions of continental scale and analyze them seamlessly for content and for change.

Raw data
(SIR-C, ERS)

Image
Formation
via computational
transforms

Image
data

Repeat Orbit Interferometer
(ROI) processing software

- Image correlation
- Interferogram generation

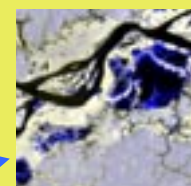
Interferograms

Technology from this Investigation forms the kernel of a distributed world accessible data and processing system that can process all the data in near real time from a projected new NASA repeat orbit interferometric SAR (InSAR) mission, exploiting its true potential.

Scientific Achievements

Amazon Rainforest Visualization/Classification project - JPL

First dual season Amazon mosaic accurately measures inundation and deforestation.

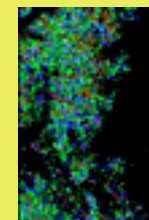


Backscatter From:
Dry Season Maps to Blue
Wet Season Maps to Red & Green

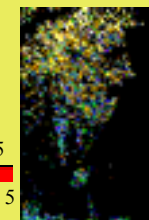
- Slate is unchanged with season
- Black is open water all year
- Yellow is inundated in wet season
- Blue is flooded in wet season only

Snow Measurement project - UCSB

Showed for the first time that multi-parameter SAR is capable of measuring the most important parameter - snow water equivalence.



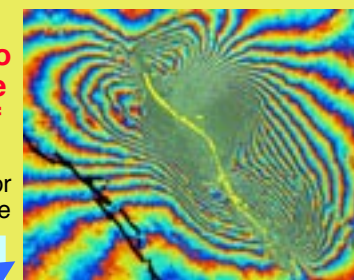
Snow
Density (left)
Depth (right)



Tectonic Deformation project - Scripps Institution of Oceanography

Scripps team developed the X-Band downlink system, when connected to high speed networks, can deliver the data for near-real time processing of events such as the Hector mine earthquake

Interferogram of Hector Mine Earthquake



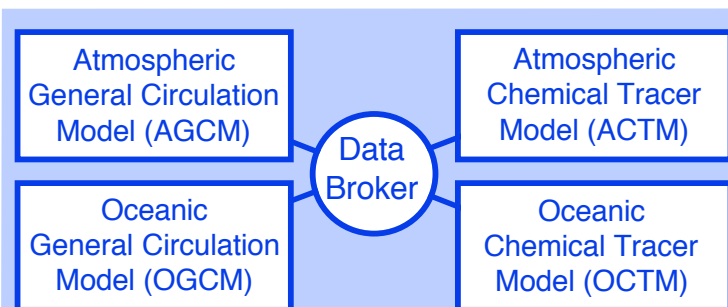


Development of an Earth System Model (ESM): Atmosphere-Ocean Dynamics and Tracers Chemistry

Carlos R. Mechoso, UCLA
<http://www.atmos.ucla.edu/esm>

Goal: Develop and apply to problems of climate change a model that describes the coupled global atmosphere - global ocean system, including chemical tracers.

Ultimate goal: Have an ESM capable of performing ensembles of century-long simulations.



UCLA Earth System Model

Developed four model elements:

- UCLA AGCM
- JPL version of LANL Parallel Ocean Program (POP)
- UCLA ACTM (which can include up to 64 species)
- JPL Ocean Chemical Transport Model

Developed the Distributed Data Broker to couple all models

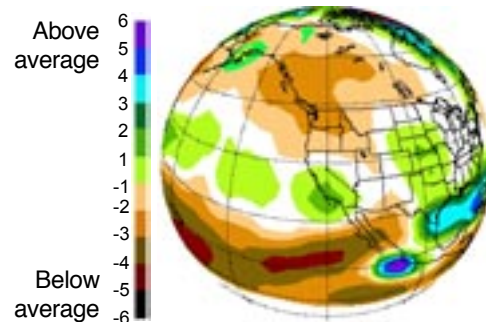
Designed each model for high performance parallel internal execution

Designed the Earth System Model for concurrent execution of models

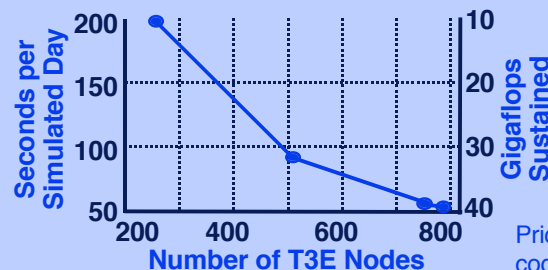
Used UCLA Earth System Model to make:

- **Realistic Simulations of El Niño-Southern Oscillation (ENSO)**
- **Decade-Long simulations of Chlorofluorocarbons (CFC-11 and CFC-12) in the Atmosphere**
- **High-resolution simulations of the Atlantic Climate (AGCM: 2.5° lon. X 2° lat. X 29 layer; OGCM: 1/6° lon. X 1/6° lat. X 37 layer)**

Predicted precipitation February-March 1998



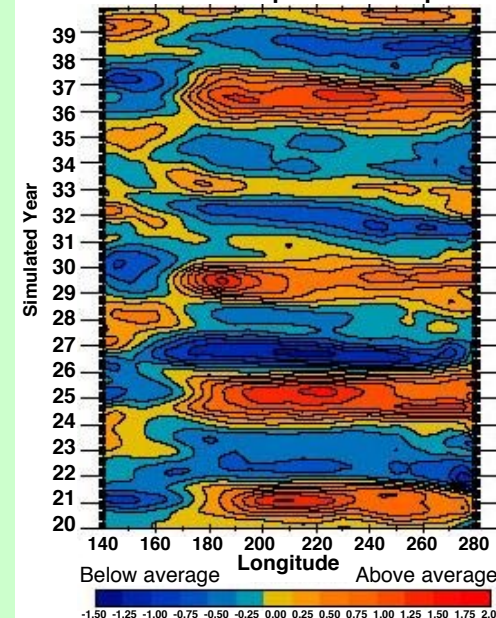
Ensemble predictions for the 1997-98 El Niño winter with the AGCM succeeded in capturing the observed evolution of climate anomalies. In parts of California, for example, predicted precipitation was only slightly above average in November-December, but more than double the average during February-March. Additional experiments demonstrated that anomalies in the Indian Ocean can impact significantly the North American winter climate. (Contour interval: 1 mm/day)



Performance of the coupled AGCM/OGCM/ACTM model on 787 processors of a CRAY T3E-600

Prior to ESS support, the precursor to these codes was baselined in 1992 at 200 megaflops.

Sea surface temperature at equator



The highly realistic ENSO produced by the coupled AGCM/OGCM was obtained through extensive model development and numerical experimentation allowed by the efficient model codes developed under this project. (Contour interval: 0.25°C)



National Aeronautics and Space
Administration

Earth Science Enterprise

Simulations Yield First Comprehensive Picture of Chlorofluorocarbons in the Atmosphere

Simulations performed on a NASA/Goddard Space Flight Center supercomputer have yielded the first comprehensive 3-D picture of the long-term evolution of chlorofluorocarbons (CFCs) in the Earth's atmosphere.

CFCs were once thought to be the perfect designer chemicals: they were cheap and did not react with anything. Only after air conditioners and spray cans ejected CFCs for decades did scientists realize they could play a major role in depleting the ozone that protects life from the sun's ultraviolet rays. When CFCs reach the stratosphere, their chlorine atoms become reactive and break up ozone molecules. Their impact includes the ozone hole over Antarctica that has been occurring every spring for the last couple of decades.

Mohan Gupta, Richard Turco, C. Roberto Mechoso, and Joseph Spahr at the University of California, Los Angeles (UCLA) recently simulated the slow emission of 20 million tons of CFCs, including the reactions that change the chemicals into ozone-eaters, over 35 years. With partial funding from NASA's Earth Science Enterprise, they were able to explore the entire global history of the two most widely used CFCs, substances known as CFC-11 and CFC-12.

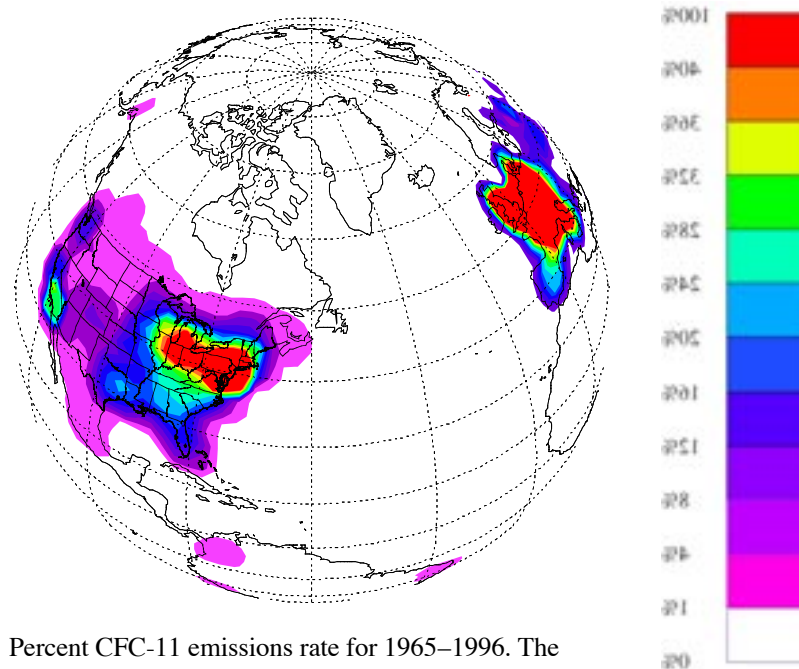
CFC usage was relatively low from 1931 until 1965, so the researchers combined emission estimates for that period and used them as starting conditions for simulations running through 2000. In full 3-D, the supercomputer kept track of emissions, CFC movements through the atmosphere, and subsequent chemical reactions every hour for 35 years. No group had ever performed such realistic simulations for so long a period.

The UCLA simulations follow for the first time the long tale of how CFCs emitted at the surface get carried by winds to remote locations up to 50 kilometers (30 miles) above the Earth. By simulating the full stratosphere rather than just the stratosphere's lower realms where most CFC break-up occurs, the team was able to significantly narrow uncertainties in CFC lifetimes. These statistics have ramifications not only for ozone depletion but also for global warming because of CFCs' greenhouse gas properties.

Validation for the simulations came from a network of eight surface observation stations scattered throughout the globe. These include the five Advanced Global Atmospheric Gases Experiment (AGAGE) stations supported by NASA and international collaborators. Simulations typically differed by just a few percentage points from each station's readings.

The cover visualization shows the concentration of CFC-11 in the lowest simulation layer (centered at around 0.22 km/0.14 miles) averaged for the northern hemispheric winter in 1990.

A paper discussing these results appears in the June 27, 2001 issue of the *Journal of Geophysical Research - Atmospheres*. The National Science Foundation also funded the study.



Percent CFC-11 emissions rate for 1965–1996. The highest emissions cluster over major industrial areas in the eastern United States and western Europe.

October 2001



Solar Activity and Heliospheric Dynamics

John Gardner, Naval Research Laboratory

<http://www.lcp.nrl.navy.mil/hpcc-ess>

Goal: To understand the engine driving space weather: the magnetohydrodynamic mechanisms of solar activity and the response of the heliosphere

CRUNCH3D

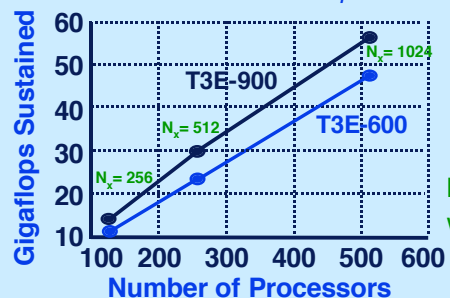
CRUNCH3D is a 3D Fourier collocation code for dissipative, compressible MHD. In this Investigation, it is applied to the evolution of magnetic flux tubes in the Solar convection zone and corona.

Round-1 and Round-2 Improvement

	1991	1998
• Performance (Gflops)	0.4	56.2
• k-space grid size enabled (reflects the number of different wavemodes included in the solution representation)	64 ³	256 ³
• Magnetic Reynolds number (physical value is of order 10 ¹⁰)	100	10,000

CRUNCH3D Performance

Problem Size Scaled with Computer Size

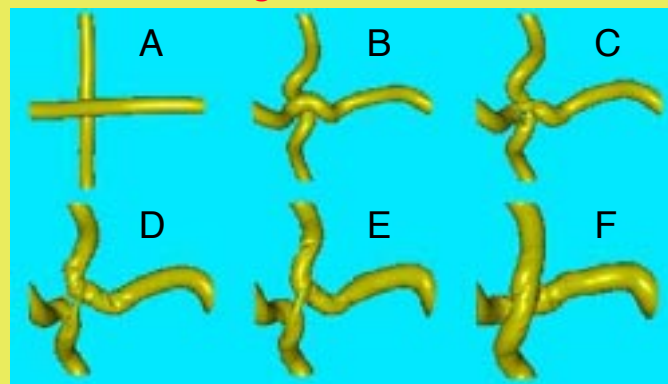


The size of the simulations enables us to clearly separate the large driving and small dissipative spatial and temporal scales.

k-space grid size = $N_x \times N_y \times N_z$
 with $N_y = 384$ and $N_z = 512$

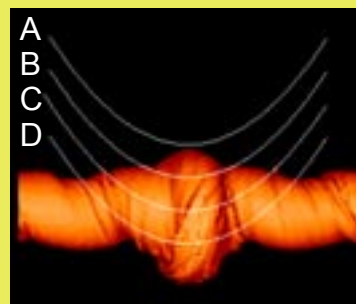
Simulations explored reconnection and kinking of buoyant magnetic flux tubes in the Solar convection zone and corona:

At the high magnetic Reynolds numbers made newly accessible under HPCC, flux tubes can 'tunnel' through each other. This remarkable behavior was wholly unanticipated theoretically, and had not previously been seen numerically in studies of magnetic flux tube interactions.

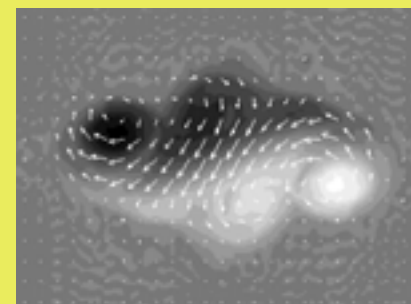


In this sequence, two flux tubes are moved together and the horizontal one appears to tunnel through the vertical one.

Demonstrated how kinking of flux tubes may explain unusual features of emerging δ -spot active regions



Isosurface of magnetic energy for an unarched flux tube with 4 mode kink.



Magnetogram as observed at time D when the flux tube on the left has arched and partially emerged through the Solar surface.



Solar Activity and Heliospheric Dynamics

John Gardner, Naval Research Laboratory

<http://www.lcp.nrl.navy.mil/hpcc-ess>

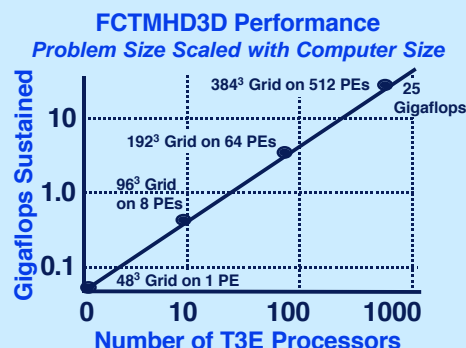
Goal: To understand the engine driving space weather: the magnetohydrodynamic mechanisms of solar activity and the response of the heliosphere

FCTMHD Suite

Flux Corrected Transport Magneto Hydrodynamics (FCTMHD) codes solve the multi-dimensional ideal MHD equations. In this Investigation, they are applied to study the evolution of magnetic fields in the Solar atmosphere.

- FCTMHD2.5D - 2-D spherical coordinates with a third component of magnetic field and fluid momentum.
- FCTMHD3D - 3-D cartesian coordinates.

PARAMESH is a parallel AMR toolkit, developed at NASA Goddard, that enables AMR for codes that use structured grids.



- Grids used range up to 512x512x512
- The size of the simulations enables us to clearly separate the large driving and small dissipative spatial and temporal scales.
- AMR maximizes simulation resolution for given fixed machine resources.

In Round-2

- Improved performance of FCTMHD3D by factor of 500 over 1992 baseline on a Cray C90.
- Added Adaptive Mesh Refinement (AMR) to FCTMHD2.5D and FCT MHD3D.

FCTMHD3D
FCTMHD2.5D

+
PARAMESH
=

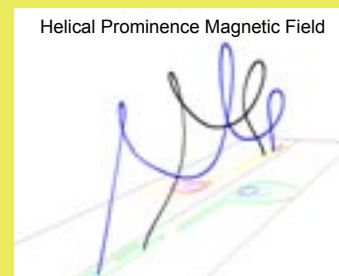
AMRMHD3D
AMRMHD2.5D

FCTMHD with AMR provided by PARAMESH is helping to develop space weather prediction tools by enabling simulations with realistic solar boundary conditions and by reducing the numerical diffusion in the direction of physical limits.

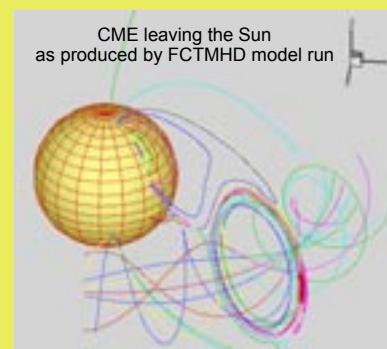
The best resolved simulations to date explored shear, reconnection, and helicity of magnetic fields in the solar atmosphere:

Uncovered a new mechanism for the formation of helical fields in Solar prominences

Helical fields were found to be a product of internal reconnections between the magnetic fields of a strongly sheared prominence and its overlying coronal arcade.
Helicity measures twistedness of magnetic field lines.



Shown quantitatively, for the first time, that non-uniform solar rotation can account for the observed rate of production of helicity in the corona.



First demonstration of the formation and complete ejection of a flux rope in a Coronal Mass Ejection (CME) based on an explosive 'breakout' of stressed magnetic flux through a restraining, overlying field.

CME was initiated by strong shearing of the field lines near the equator at the inner solar boundary. CME flux rope leaves the inner corona at approximately 1000 km/sec.



Turbulent Convection and Dynamos in Stars

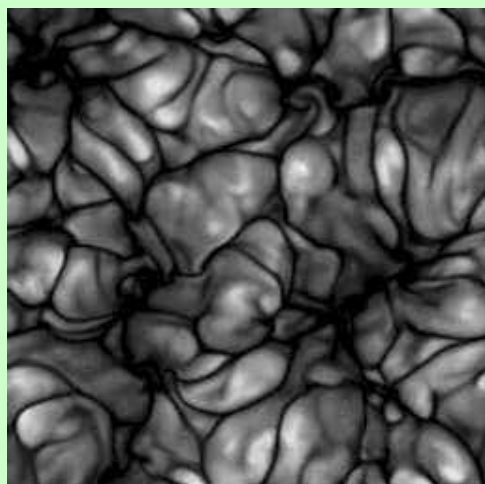
Andrea Malagoli, University of Chicago
<http://astro.uchicago.edu/Computing/HPCC/>

Goal: *To understand the structure and evolution of both large- and small-scale magnetic fields near the surface of the Sun.*

For the first time the resolution of simulations of turbulent convection on the Sun's surface can exceed the resolution of the observations.

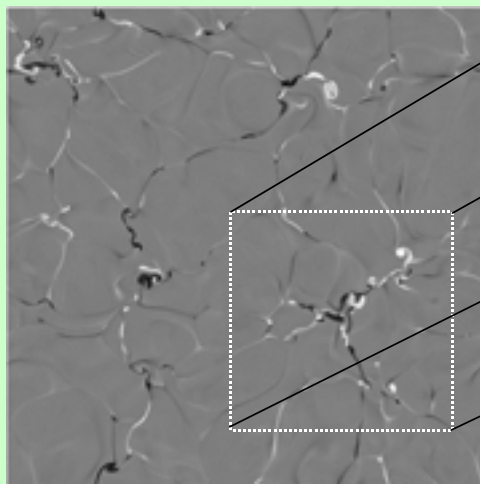
- Provides an important framework for the analysis of observations by eliminating incorrect interpretations.
- Provides robust theoretical guidelines for the planning of future missions like Solar-B.

Temperature of top layer

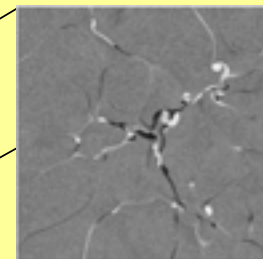


Light color represents hotter fluid moving up out of the page; dark color represents colder, sinking fluid.

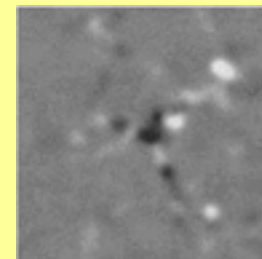
Magnetic Flux of top layer



Light color represents large positive flux pointing up out of the page; dark color represents large negative flux.



"actual" distribution produced by simulation

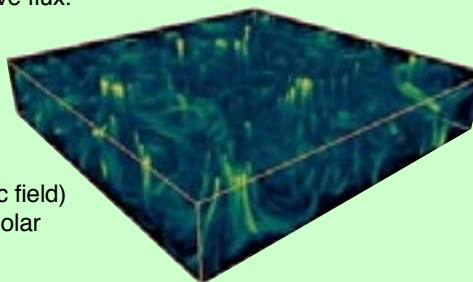


"blurred" distribution that would be observed by an instrument. It may be interpreted incorrectly as an emerging coherent flux tube.

Results from MPS, a MHD PseudoSpectral code simulating magnetic fields in the Sun

- Carried out on a 512x512x97 grid.
- The size of the simulation enables it to contain several coherent structures that can be associated with the sun's granules.
- Run at 50 GigaFlop/s on 512 processors of the ESS Cray T3E at GSFC.
- 100,000 iterations

Magnetic enstrophy
(the square of the magnetic field)
near the surface of the solar
convection zone





Relativistic Astrophysics and Gravitational Wave Astronomy

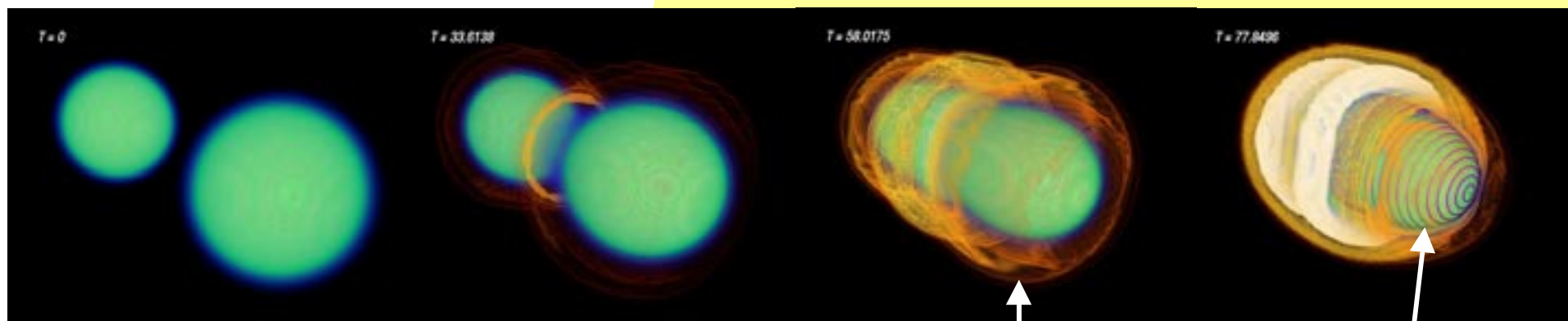
Paul Saylor, University of Illinois

<http://wugrav.wustl.edu/Relativ/nsgc.html>

Goal: *Combine fluid dynamics and General Relativity to investigate the merger of two neutron stars, a process that encompasses many aspects of relativistic astrophysics.*

For the first time, Neutron Star mergers are being simulated using Einstein's theory of General Relativity

Calculations using the fully relativistic model of gravity, as opposed to previous calculations using the post-Newtonian approximation, **reveal that a Black Hole can result from such a merger.**



In this calculation, two Neutron Stars, each having 1.4 solar mass, collide head-on and merge to form a Black Hole.

Visualization by: Werner Benger and the NCSA/Potsdam/Wash.U/ZIB visualization team
Simulation by: Mark Miller and the Washington University/Albert Einstein Institute neutron star team, the NASA Neutron Star Grand Challenge Collaboration.

Shock waves of heated gas generated by the collision.

The *Horizon* - inside this surface, the pull of gravity is so strong that even light collapses.

Results produced by GR3D, a 3-D General Relativity code coupling the Einstein Equations and relativistic hydrodynamic equations

- Computation carried out on a 160x160x160 grid run for 3000 time steps.
- Run at 25 GigaFlop/s sustained for 30 hours (totaling 100 trillion floating point operations) on 512 processors of the ESS Cray T3E at GSFC.
- GR3D couples multidisciplinary codes using the Cactus framework [<http://cactus.aei-potsdam.mpg.de/index.html>].

Future: extend simulations to compute signatures of gravity waves emitted by Neutron Star mergers to support gravitational wave observatories being built in the U.S. by the LIGO project and in Europe by the VIRGO and GEO projects.



Multiscale Modeling of Heliospheric Plasmas

Tamas Gombosi, University of Michigan

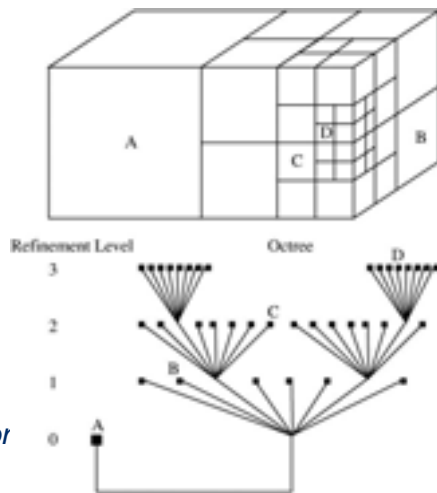
<http://hpcc.engin.umich.edu/HPCC/>

Goal: To accurately simulate the dynamic Heliosphere, propagating the solar wind from the surface of the Sun to the interstellar shock for a complete solar cycle.

Simulation performed using Block Adaptive Tree Solar-wind Scheme code (BATS-R-US)

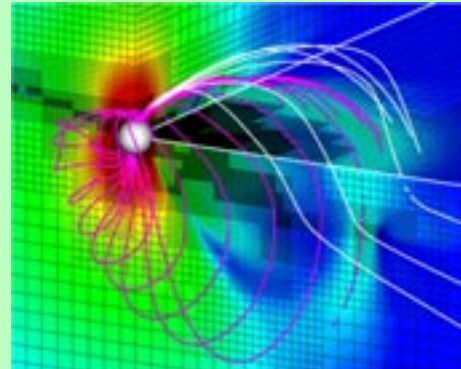
BATS-R-US is:

- Cell-centered upwind finite volume formulation with high-resolution Godunov-type scheme.
- Block-based Adaptive Mesh Refinement (AMR):
 - Physics-based refinement and coarsening criteria
 - Resolution of multiple solution scales
- Parallel implementation:
 - Multiscale domain decomposition
 - Portable implementation (FORTRAN90/MPI)
 - Achieved 345 Gflops on a 1,490 processor Cray T3E-1200 with near-perfect scalability
 - Simulation ran for 80 hours on 512 processors. This was about 50% faster than real time (the simulation time was 125 hours).

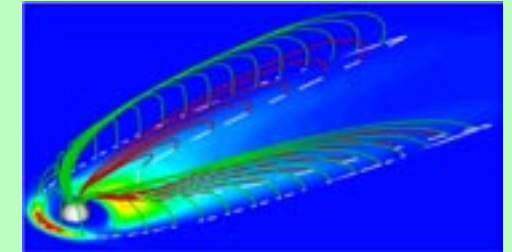


First ever “Sun to Mud” Space Weather Simulation

Generation of a Coronal Mass Ejection (CME), its interplanetary propagation and its interaction with the Earth’s magnetosphere-ionosphere system.

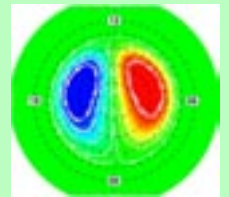


CME near the Sun 9-hours after its initiation



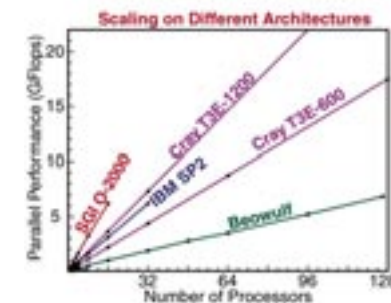
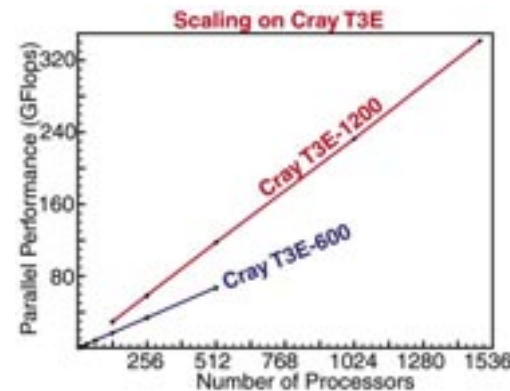
Magnetosphere of the Earth interacting with the CME;

and the corresponding ionosphere



Other Applications of BATS-R-US:

- Solar wind interaction with planets and comets.
 - Solar wind interaction with Mercury, Venus, Mars and Saturn
 - Solar wind interaction with comets and simulation of cometary x-rays
- Interaction of planetary satellites with planetary magnetospheres.
 - Interaction of Io and Europa with Jupiter’s magnetosphere
 - Titan’s interaction with Saturn’s magnetosphere

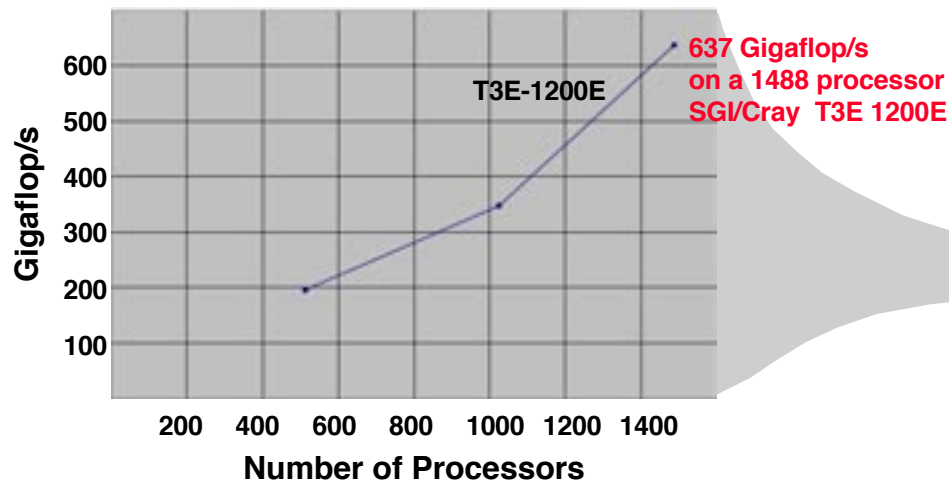




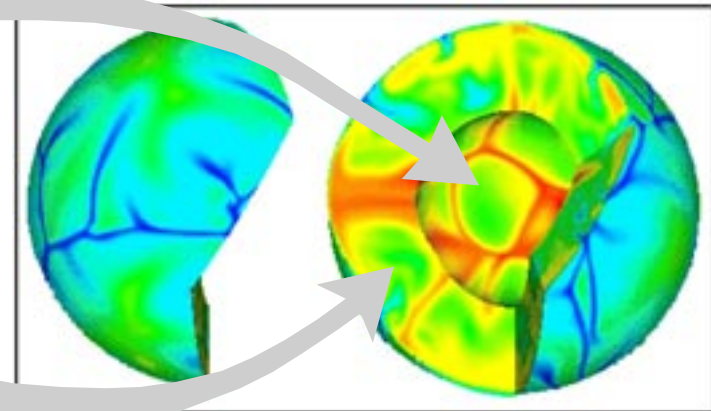
Three-Dimensional Spherical Simulations of Earth's Core and Mantle Dynamics

Peter Olson, Johns Hopkins University, Principal Investigator
<http://curie.eps.jhu.edu/nasa3/start.html>

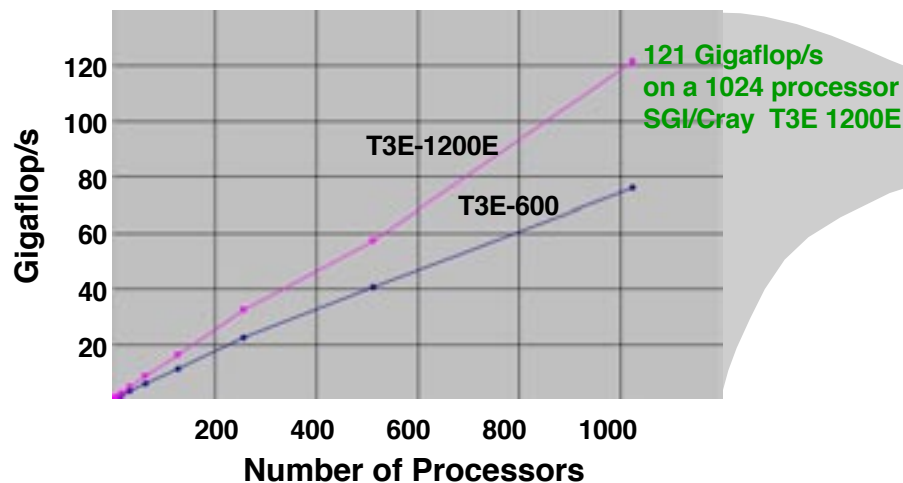
DYNAMO Performance



DYNAMO is a 3-D code for studying the Earth's magnetic dynamo which arises from the turbulent convective processes in the Earth's core. This code solves the full anelastic magnetohydrodynamic (MHD) equations in a spherical geometry using pseudospectral (spherical harmonic expansion) methods.



TERRA Performance



TERRA is a 3-D spherical finite element mantle dynamics code which treats the silicate material that comprises the Earth's mantle as a (non-linear) viscous fluid and solves the Navier-Stokes equations in 3-D spherical geometry for the motions that arise due to the temperature and density variations.



PARAMESH - Parallel Adaptive Mesh Refinement (AMR) toolkit

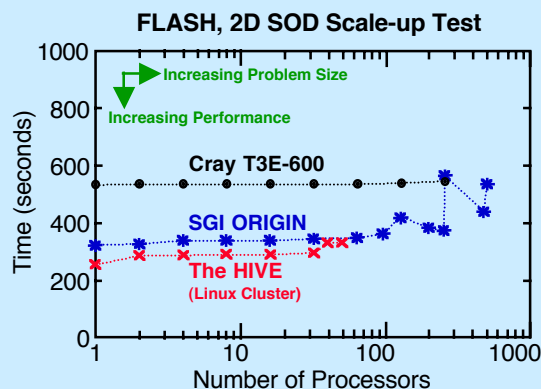
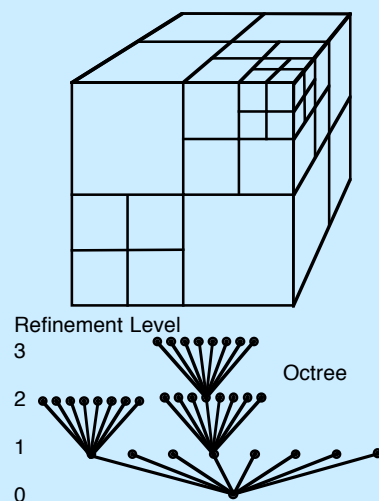
http://sdcd.gsfc.nasa.gov/RIB/repositories/inhouse_gsfc/Users_manual/amr.html

Goals: *Enable application developers to:*

- *Convert non-AMR structured codes to AMR*
- *Convert serial codes to parallel*

PARAMESH Features:

- Supports multi-dimensional user applications that compute on logically cartesian meshes.
- Grid size and number of refinement levels limited only by computational resources of machine.
- Highly Parallel
- Scalable (latency tolerant)
- Portable (MPI, SHMEM)
- Works for structured grids
- Builds on users' existing codes
- User tunable load balancing
- User provides criteria for refining blocks
- Written in Fortran 90
- Open source software
- Users manual in HTML



Development Team:

Peter MacNeice
GSFC and Drexel Univ.
Kevin Olson
GSFC and U. of Chicago

Chief Customers:

University of Chicago

DOE ASCI FLASH Center Code Group

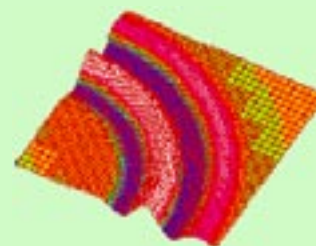
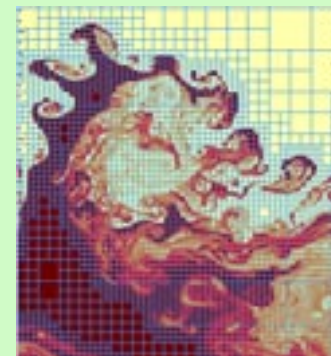
General astrophysical applications

<http://flash.uchicago.edu/>

2000 Gordon Bell Award winner:

"Simulation covered both the largest domain and the finest spatial resolution ever conducted for this type of calculation"

<http://sc2000.org/awards/index.htm>



Drexel University

General Relativity (GR) Group

Modeling GR wave signatures from interacting compact objects

<http://einstein.drexel.edu/>

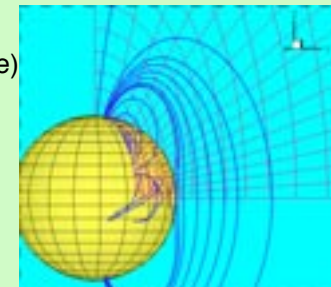
First evolution of pure gravitational waves using AMR in the full Einstein equations.

Naval Research Laboratory (NRL)

Solar Physics Group (ESS Round-2 Awardee)

MHD modeling of the solar atmosphere and Space Weather

<http://www.lcp.nrl.navy.mil/hpcc-ess/>



Other Customers:

Naval Research Laboratory

Ionospheric Modeling Group

GSFC, Code 695

- MHD modeling of solar wind and the magnetosphere

University of Catania, Italy

- Hydrodynamic modeling of the solar corona



Ensemble Calculations for Seasonal Forecasting

Max Suarez/GSFC, NASA Seasonal to Interannual Prediction Project (NSIPP)

<http://nsipp.gsfc.nasa.gov/>



Goal: *Establish the degree to which clusters of PC's may reduce the cost of ensemble forecasting.*

For the NSIPP atmospheric model, a cluster of commodity PC's provides performance similar to commercial products, but at significantly lower cost.

Computation of one simulated day using a 288x180x22 grid run on 32 processors of:

Cray T3E-600



Requires:

20 minutes

Origin 2000



10 minutes

theHive (Linux cluster of PCs)



29 minutes

The 32 processor Linux cluster cost \$120K in mid 1999, making it roughly 3 times more cost effective than the Origin.

The PC cluster approach is now commercially offered. It allows the latest PC chips to be made available in the computing center for high end applications as soon as they are available to the public.

Creation of the Linux cluster: John Dorband/GSFC

Porting to the Linux cluster: Tom Clune/SGI

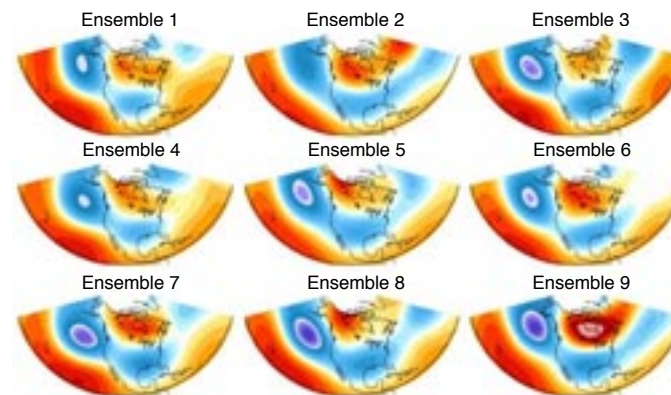
Porting to the Origin: Jim Abeles/SGI, Tom Clune/SGI

Timing on the T3E: Max Suarez/GSFC

Since ensemble members are independent they can be run in parallel. 18 runs, using 32 processors each, would efficiently utilize 576 processors. Such work can be done cost effectively on 18 small clusters, reserving large, tightly coupled supercomputers, such as the T3E, for tasks in which independent calculations cannot be so readily organized.

Results produced by NSIPP atmospheric model

Forecast anomalies of the upper level flow of the 1983 El Nino event.



The panels show nine realizations taken at random from an 18-member ensemble forecast. Anomalies over North America are very similar in all members. Over the North Atlantic, however, there is considerable random variability. Ensemble forecasts are required to distinguish between these situations.